A New Online Computer Program for Neutron Activation Analysis

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Purpose: Neutron Activation Analysis (NAA) is a highly sensitive, non-destructive radioanalytical method used to identify and quantify major, minor, and trace elements across various materials. This technique works by bombarding a sample with neutrons, triggering nuclear reactions that transform stable nuclei into radioactive ones. By analyzing the unique gamma-ray spectra emitted by these product nuclei, the elemental composition can be accurately determined (Greenberg et al., 2011). Despite its precision, the post-irradiation phase-encompassing peak extraction, isotope identification, and concentration calculations-is often complex, labor-intensive, and susceptible to human error. To overcome these limitations, we have developed the Nuclear Activation Analysis System (NAAS), an integrated online platform that automates and streamlines the entire data analysis workflow.

Methods: The widely used method of NAA for determining elemental concentrations in samples is the direct comparator method, in which a reference material (indexed as R) containing a known amount of the element(s) of interest is irradiated together with the sample (indexed as S) and counted under identical geometric conditions (Greenberg et al., 2011). According to classical neutron activation theory (Nangeelil et al., 2023), the relationship between the mass of the element x in the sample ($m_{x,S}$) and net peak area of spectra (P_s) is:

$$m_{x,S} = C_s m_s = P_s \cdot \frac{M_a}{N_{av}\theta} \cdot \frac{\lambda}{\phi_{th}\sigma_{eff} I\varepsilon(1-e^{-\lambda t_i})e^{-\lambda t_{d,s}}(1-e^{-\lambda t_{c,s}})} \#(1)$$

where C_S is the element concentration in the sample, P is the net peak area (after background subtraction); M_a is the atomic mass; N_{av} is the Avogadro's number; θ is isotopic abundance of the target isotope; λ is the decay constant of product isotope; Φ_{th} is the thermal neutron flux, σ_{eff} is the effective neutron cross-section, I is the probability of a disintegrating nucleus emitting a photon of E_γ, ε is the detector efficiency at E_γ, t_i is the irradiation time, t_d is decay time, and t_C is the counting time for the spectra collection.

The mass of the element x of interest in the reference (m_{xR}) is:

$$m_{x,R} = C_R m_R = P_R \cdot \frac{M_a}{N_{av}\theta} \cdot \frac{\lambda}{\phi_{th}\sigma_{eff} I\varepsilon(1-e^{-\lambda t_i})e^{-\lambda t_{d,R}}(1-e^{-\lambda t_{c,R}})} \#(2)$$

We supposed the neutron flux is the same in sample and reference, then divide Equations (1) and (2), we get:

$$C_S = C_R \cdot \frac{P_S}{P_R} \cdot \frac{m_R}{m_S} \cdot \frac{e^{-\lambda t_{d,R}}}{e^{-\lambda t_{d,S}}} \cdot \frac{1-e^{-\lambda t_{c,R}}}{1-e^{-\lambda t_{c,S}}} \#(3)$$

Corresponding concentration uncertainties were calculated using standard error propagation equation as below. $\Delta C_S = C_R \cdot \sqrt{\left(\frac{\Delta C_R}{C_R}\right)^2 + \left(\frac{\Delta P_S}{P_S}\right)^2 + \left(\frac{\Delta P_R}{P_R}\right)^2 + \left(\frac{\Delta m_R}{m_R}\right)^2 + \left(\frac{\Delta m_S}{m_S}\right)^2}$ #(4)

These calculations were integrated into the proposed NAAS. For more convenient retrieval of nuclide property information, the system also integrates multiple databases, including atomic weights and isotopic compositions for all elements, search for radionuclides, gamma energy lines search, and data for commonly used standard reference materials. These data are compiled from sources published by NIST and other recognized laboratories (Coursey et al., 2015; Glascock, 2015).

NAAS is designed and implemented using SQL for structured data storage, PHP for database access and data visualization, and Python for data processing, analysis, and program execution, and web-based interface development. An automated module was added to identify and extract experimental data from Genie 2000 output files. Genie 2000 is a nuclear spectroscopy software used for the acquisition and analysis of gamma-ray spectra (Figure 1). The extracted data include spectral peak areas, corresponding energies, and energy uncertainties required for subsequent concentration calculations. Energies obtained from Genie 2000 were compared with those in the NAAS database. If the measured energy ± its uncertainty

fell within the database energy within the preset tolerance, the data were accepted; otherwise, they were discarded. The data mapping and availability logic are shown in Figure 2.

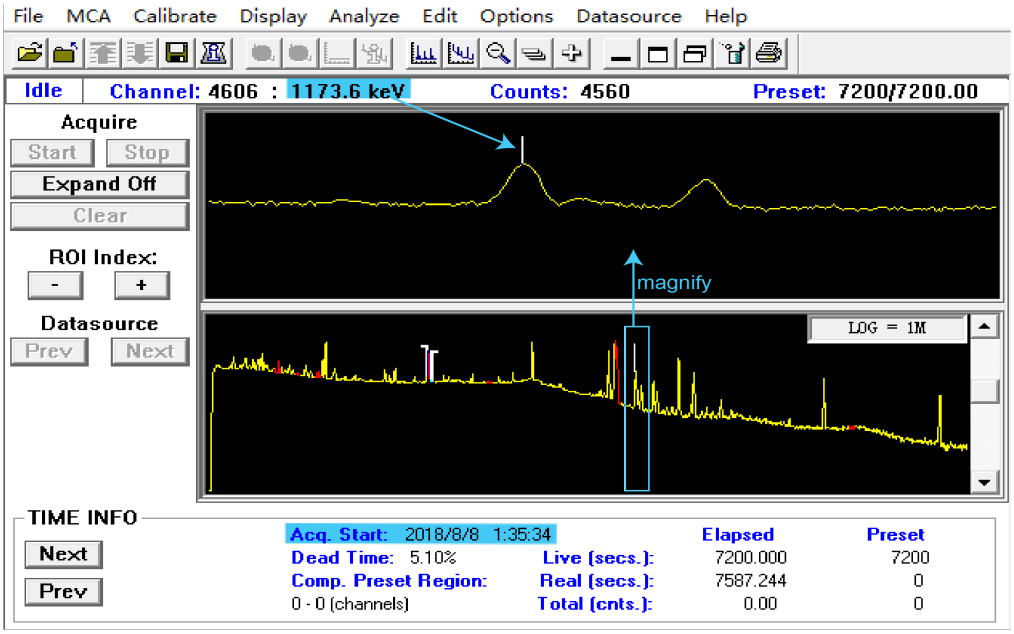

Figure 1. Interface of Genie 2000 software.

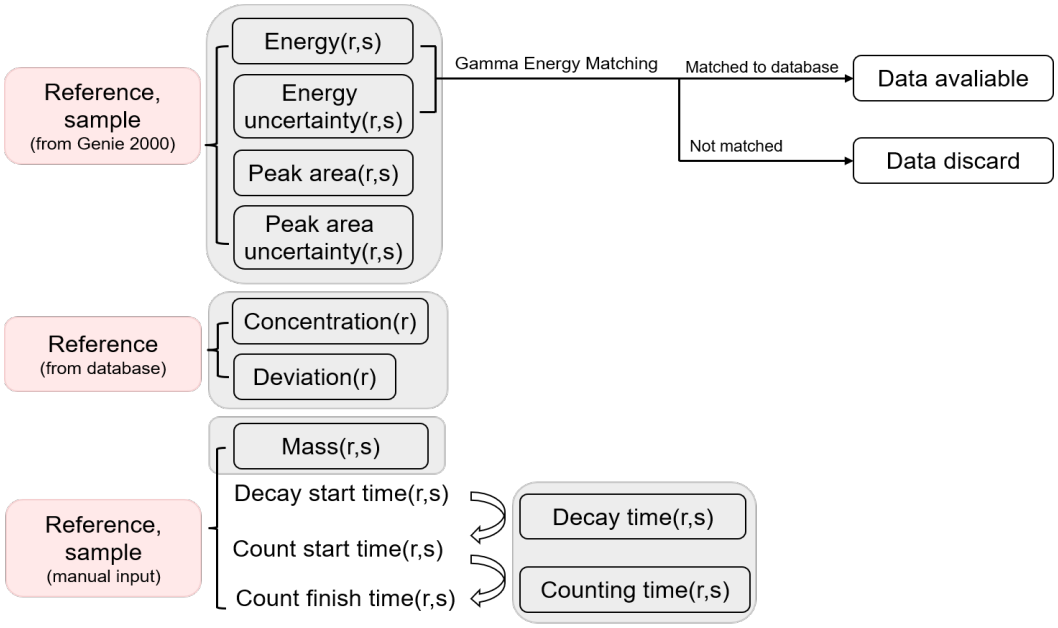

Figure 2. Data mapping and availability logic.

Results: We developed NAAS, an online platform hosted on the university's Linux server (http://neutron.research.unlv.edu, Figure 3). The NAAS provides three primary functions: (1) Retrieval of nuclide properties and nuclear reaction data relevant to NAA. By entering a nuclide name, the system performs a fuzzy search of the databases to retrieve the corresponding nuclide information and associated nuclear reactions that produce characteristic gamma-ray lines (Figure 4). (2) Automated identification and extraction of experimental data from Genie 2000. (3) Automated calculation of elemental concentrations and their corresponding uncertainties. The reliability of the system has been validated using previously acquired experimental data.

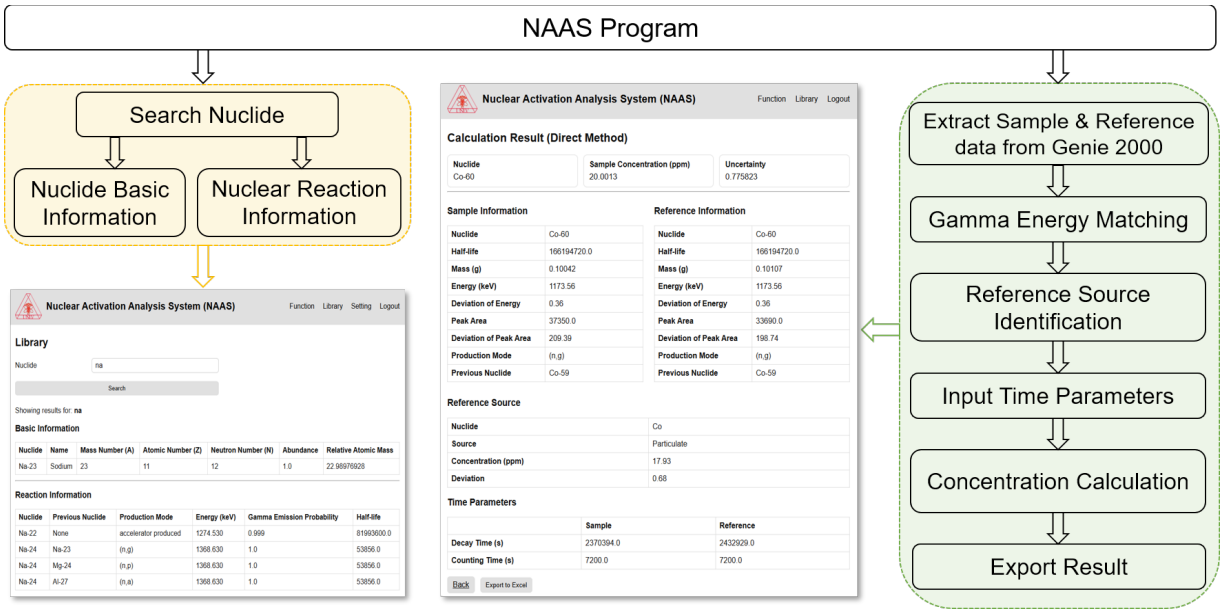

Figure 3. Workflow of NAAS.

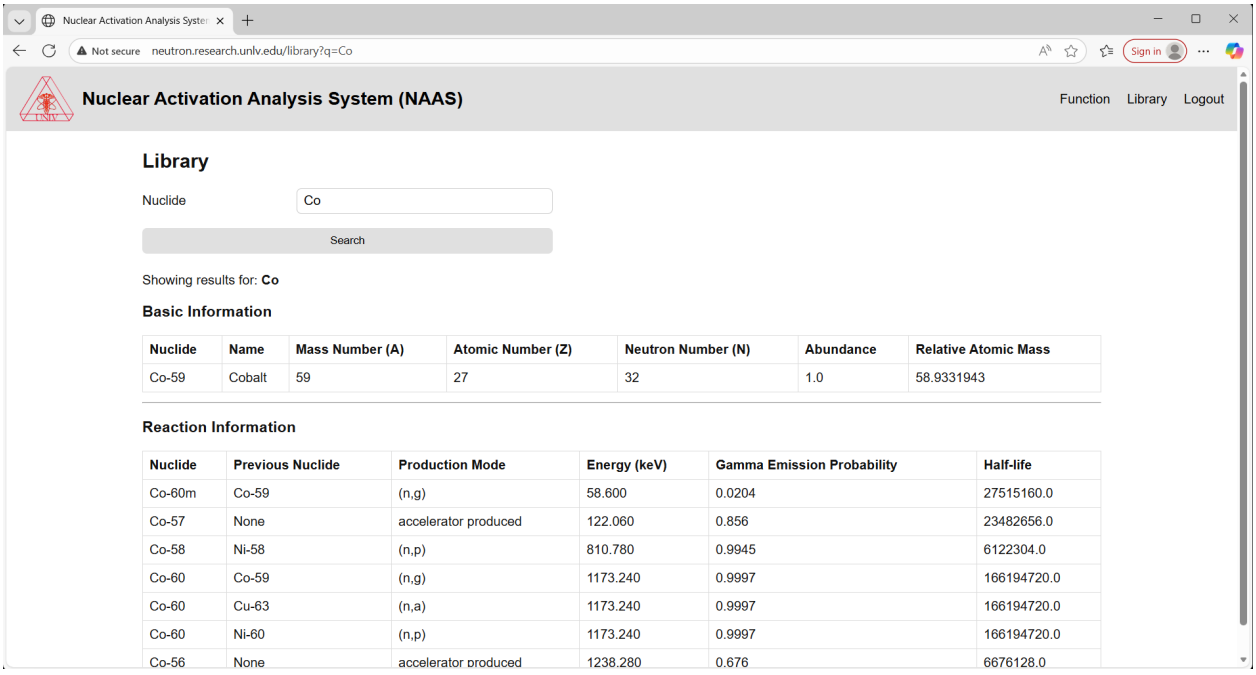

Figure 4. Library Search Interface of NAAS.

Conclusions: This project successfully developed the NAAS, a user-friendly online platform designed for calculations related to NAA. Following NAA experiments, NAAS supports batch identification of spectral peaks, automated calculation of elemental concentrations, and direct result export. The system significantly reduces labor requirements and minimizes potential human error. It is particularly valuable for users who wish to apply neutron activation analysis but may not be familiar with the underlying nuclear reactions or activation calculations. Future work will focus on incorporating additional calculations and functions, including the k_0 method and the quasi-absolute method, and S-value calculations for radioisotopes.

Relevance to CIRMS: This work is a subset of the first author's doctoral research and focuses on neutron activation calculations for samples/standards irradiated in a nuclear reactor. It aligns with the CIRMS mission, as nuclear reactors are the primary method for neutron activation of samples/ standards, and the resulting radioactivity and gamma emissions are essential for understanding isotope composition and reconstructing the 3D spatial distribution of radioisotopes. In addition, the developed software enables pre-irradiation estimation of induced activity, improving experimental planning and radiation safety. The first author aims to pursue a career as a medical physicist and currently works in a research group specializing in neutron activation analysis and 3D isotopic image reconstruction using gamma emission computed tomography.

References

Coursey, J. S., Schwab, D. J., Tsai, J. J., & Dragoset, R. A. (2015). *Atomic Weights and Isotopic Compositions (version 4.1).* http://physics.nist.gov/Comp, accessed on 02/15/2026.

Glascock, M. D. (2015). Tables to Support the Analytical Methods in Use at MURR: NAA, XRF and ICP-MS. *Research Reactor Center, University of Missouri, Columbia, 65211.*

Greenberg, R. R., Bode, P., & De Nadai Fernandes, E. A. (2011). Neutron activation analysis: A primary method of measurement. *Spectrochimica Acta Part B: Atomic Spectroscopy, 66(3–4), 193–241.* https://doi.org/10.1016/j.sab.2010.12.011

Nangeelil, K., Dimpfl, P., Mamtimin, M., Huang, S., & Sun, Z. (2023). Preliminary study on forgery identification of Hetian Jade with Instrumental Neutron Activation Analysis. *Applied Radiation and Isotopes, 191, 110535.* https://doi.org/10.1016/j.apradiso.2022.110535